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RADIONUCLIDE DAUGHTER INVENTORY GENERATOR CODE: DIG

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ABSTRACT

The Daughter Inventory Generator (DIG) code accepts a tabulation of radionuclides initially present in a waste stream, specified as amounts present either by mass or by activity, and produces a tabulation of radionuclides present after a user-specified elapsed time. This resultant radionuclide inventory characterizes wastes that have undergone daughter ingrowth during subsequent processes, such as leaching and transport, and includes daughter radionuclides that should be considered in these subsequent processes or for inclusion in a pollutant source term. Output of the DIG code also summarizes radionuclide decay constants.

The DIG code was developed specifically to assist the user of the PRESTO-II methodology and code (Fields et al., in press; Little et al., 1981; Fields, Little, and Emerson, 1981) in preparing data sets and accounting for possible daughter ingrowth in wastes buried in shallow-land disposal areas. The DIG code is also useful in preparing data sets for the PRESTO-EPA code [USEPA, (in press)]. Daughter ingrowth in buried radionuclides and in radionuclides that have been leached from the wastes and are undergoing hydrologic transport are considered, and the quantities of daughter radionuclides are calculated. Radionuclide decay constants generated by DIG and included in the DIG output are required in the PRESTO-II code input data set.

The DIG code accesses some subroutines written for use with the CRRIS system (Baes and Miller, 1981, 1984) and accesses files containing radionuclide data compiled by D. C. Kocher (Kocher, 1981).

1. INTRODUCTION

PRESTO-II (Prediction of Radiation Exposures from Shallow Trench Operations) is a methodology and computer code (Fields et al., in press; Little et al., 1981; Fields and Emerson, 1984; Fields, Little, and Emerson, 1981) designed to generate a radionuclide source term, simulate environmental transport, and evaluate possible health effects caused by radionuclide releases from shallow, radioactive-waste disposal trenches and from associated areas contaminated by operational spillage. This model is designed to simulate transport of radionuclides from a disposal site and to predict radionuclide exposures and cancer risks for the 1000-year period following the end of burial operations. PRESTO-II is a versatile methodology for calculating risks to local and intermediate-range populations resulting from waterborne and airborne radionuclides. The DARTAB code (Begovich et al., 1981) is used by PRESTO-II as a subroutine to combine simulated radionuclide exposure values with dose and health risk factors to produce tabulations of dose and health risk. PRESTO-II has been used to evaluate the consequences of disposing of de minimis levels of radioactive wastes (Fields and Emerson, 1984), and is supported by a data set generator code, PRESTO-PREP (Bell et al., 1984). The PRESTO-PREP code accesses both nuclide- and risk-specific data to prepare PRESTO-II data sets.

Near-surface transport mechanisms considered in the PRESTO-II methodology are trench cap failure, cap erosion, farming or reclamation practices, human intrusion, chemical exchange within an active soil layer, contamination from trench overflow, and dilution by surface streams. Subsurface processes include infiltration and drainage into the trench, the ensuing dissolution of radionuclides, and chemical exchange between trench water and buried solids. Mechanisms leading to contaminated water outflow include trench overflow and downward vertical percolation. If the latter outflow reaches an aquifer, the model considers radiological exposure resulting from drinking contaminated water and from irrigation and subsequent ingestion.

Radionuclide decay is accounted for in the PRESTO-II code, but daughter ingrowth in the burial area and during transport is not specifically included. (The effects of daughter ingrowth after

inhalation or ingestion is, however, considered.) The PRESTO-II user must include in the input data set entries for daughters arising during trench residence or transit.

The DIG (Daughter Generator Code) code has been written to assist the PRESTO-II user in preparing an input data set that properly considers daughter ingrowth. The DIG code accepts a tabulation of radionuclides initially present in a waste stream, specified as amounts present either by mass or by activity, and produces a tabulation of radionuclides present after a user-specified elapsed time.

DIG output lists daughter radionuclides that would ingrow, together with their activities, based on the initial quantities of the parent radionuclides and the elapsed time. The output also lists amounts of parent radionuclides remaining and summarizes the radionuclide decay constants needed for PRESTO-II input. These values may be used in manually preparing a PRESTO-II data set or as input to the PRESTO-PREP code mentioned previously.

2. DESCRIPTION OF DIG METHODOLOGY AND CODE STRUCTURE

The DIG code accesses certain subroutines written for use with the CRRIS system (Baes and Miller, 1981, 1984) and accesses radionuclide data compiled by D. C. Kocher (Kocher, 1981). The DIG methodology may be operationally summarized in three steps:

- Step 1: DIG reads the user-specified nuclides initially present in the waste. DIG will invoke the PRIMUS code (one of the suite of models of CRRIS) (Hermann et al., 1984), to generate the radionuclide decay chain and a matrix of decay coefficients. This will be referred to as the PRIMUS data set.
- Step 2: Using either element-specific masses (kg) or activity (Ci) values supplied by the user, DIG converts the amounts of initial nuclides present to units of activity and reads the nuclide-specific decay parameters from the PRIMUS data set generated in step 1.
- Step 3: Finally, DIG invokes DECAVC (also a submodel of CRRIS) which calculates the amounts of daughter radionuclides present after the specified time has elapsed. DIG summarizes the radionuclide inventory present and prints the results, together with the radionuclide decay constants, for use in the PRESTO-II input data set.

These steps are executed as a multi-step computer job using the FORTRAN programs included in Appendix A and the job control language of Appendix B. Appendix C contains an example calculation.

Appendix D contains a FORTRAN listing and the job control language for using DCHAIN, a program which may be used to unpack (from compressed data format) and display the PRIMUS data set generated in Step 1 above. This program is included as a convenience to those who may wish to make use of the radionuclide data set in other applications.

3. CODE USAGE

The DIG code is most easily used by preparing a submission file containing job control language, such as that included in Appendix B.1, and submitting a multistep job. All data input to DIG is done through NAMELIST reads.

The normal sequence for using DIG is to create a PRIMUS data set by using NAMELIST CONST which defines the number of parents, NUMREL. See Appendix B.1 for the NAMELIST data. Note that there may be only one member in a chain. Associated with NUMREL is the name of each parent which is entered in NAMELIST NAMES. The name of a radionuclide is a literal string of the form "U-238" with no embedded blanks and a hyphen between symbol and mass. For most applications, the values of parameters LBMODE and SEDIT will be zero, as shown here. The effect of choosing other values for these control parameters is discussed elsewhere (Hermann et al., 1984). The first step, S1 in Appendix B.1, is the PRIMUS step which sets up the decay matrix for the parents and associated daughters on logical unit 14.

When the second step (S2 of Appendix B.1) is executed, DIG reads the decay matrix from the PRIMUS data set (FT14F001) created in S1 and reads the initial type (CI or KG) into array TYPE and quantity into array QUANT from NAMELIST ACTIV. These parameters must be in the same order as in the RELSYM array in S1. Parameter INTERM when greater than 0 indicates that the intermediate table of radionuclides is desired and TB is the user-specified time for decay in years. DIG can be used to study the effect of specific releases or occurrences of radionuclides by setting INTERM greater than zero. The intermediate table (INTERM>0 in NAMELIST ACTIV) shows the activities after TB years of each of the members of a chain, without combining any duplicate nuclides within the total list of nuclides. The occurrence of a nuclide can therefore be traced back to a particular source.

The user does not have to use all steps as outlined in Chapter 2. For example, the user may decide that he has miscalculated the initial activity of a nuclide, but he does not have to rerun the first step in the JCL (Appendix B.1). The user may start with the already created PRIMUS data set and correct the appropriate activity or mass in NAMELIST

ACTIV. The list of radionuclides does not change, and the use of DIG can utilize the JCL in Appendix B.2 for this application. The time of decay (TB) has been changed from 10 to 20 years in NAMELIST ACTIV in the JCL in Appendix B.2. The example output in Appendix C.1 corresponds to the JCL in Appendix B.1, and likewise the output in Appendix C.2 corresponds to Appendix B.2.

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Appendix A

DIG Code Listing

Appendix A. DIG Code Listing

```

C      COMPUTER PROGRAM DIG : DAUGHTER INVENTORY GENERATOR
C      NOTE:  FOR NUCLIDES WITH HALF-LIFE < 0.4 SEC,
C              VALUES WERE SAVED AS LAM'S BECAUSE
C              LAM FOR THESE NUCLIDES WERE NOT SAVED
      LOGICAL*1 EXCITE,BLANK,METAS
      LOGICAL KG,TYPE
      INTEGER ZAS,A,Z
      REAL*8 SYMK,SYMJ
      REAL LAMI
      COMMON/LAMBDA/LAMI(200)
      COMMON/TIMECN/TIME,ICTYP,ISTYP,IMULT,IDIAG,NPRIME,NOONC,
1      KOUT,NREL,NEXP,KTRUNC,NPACK
      DIMENSION HL(200),CRATE(200),INDS(200)
      DIMENSION SYN(200),IMASS(200),EXCITE(200),IANO(200)
      DIMENSION CPACK(200),VELD(200),IC(200),JC(200),S(37,37),
1      JINL(200),ZAS(200),CONC(200),DUMMY(200),VRATE(200)
      DIMENSION N1(200),N2(200),IW(200),QUANT(200),TYPE(200)
      NAMELIST / ACTIV/ TYPE,QUANT,INTERM,TB
      DATA IW/200*0/,IR/0/,CONC/200*0.0/,JCB/-1/
      DATA METAS/'M'/,BLANK/' '/,KG/'KG'/
C      ICUT IS THE LOGICAL UNIT NUMBER FOR WRITTEN OUTPUT
      ICUT=3
C      NPRIME IS THE LOGICAL UNIT NUMBER FOR THE PRIMUS DATA SET
      NPRIME=14
C      *****
C      SET PARAMETERS FOR DECAYC
      IDIAG=0
      ICTYP=0
      IMULT=0
      ISTYP=2
C      *****
C      *****
C      SET TIME CONSTANTS
      SECDAY=8.64E+04
      DAYSyr=365.2422
      SECSYr=SECDAY*DAYSyr
C      *****
C      *****
C      READ RADIONUCLIDE PARAMETERS FROM THE PRIMUS DATA SET
C      AND PROCESS FOR TABULAR OUTPUT
      REWIND NPRIME
      READ(NPRIME)NUMCHA,KTYPE,NPACK
      READ(NPRIME)(IC(N),N=1,NPACK),(JC(I),I=1,NPACK)
      READ(NPRIME)
      READ(NPRIME)NREL,NEXP,(N1(J),J=1,NREL),(N2(I),I=1,NEXP)
      NE=0
      DO 30 ICHAIN=1,NUMCHA
      READ(NPRIME)L,LQ,EX,NREL,KSHORT,JSHORT,

```

```

1 ((S(J,I),J=1,L),I=1,L),(JINL(K),K=1,NCPFL),
2 (DUM1,L1=1,L),LOUT,DUM1,(DUM2,L2=1,L),
3 (DUM1,DUM2,L3=1,LOUT),(DUM1,L4=1,L),
4 NX,((DUM1,N1=1,NX),M1=1,L),KID,JID,DLANK,DLAMU,SYMK,SYMU
DO 20 IN=1,3.
  NE=NE+1
  IF(KSHORT.NE.IN.AND.JSHORT.NE.IN)GO TO 10
  DUMMY(NE)=S(IN,IN)
  NE=NE+1
  IF(KSHORT.EQ.IN)DUMMY(NE)=DLANK
  IF(JSHORT.EQ.IN)DUMMY(NE)=DLAMU
  GO TO 20
10 CONTINUE
  DUMMY(NE)=S(IN,IN)
20 CONTINUE
30 CONTINUE
C   CREATE ZAS ARRAY TO HOLD ZAS NUMBERS FOR EXPANDED
C   NUCLIDE LIST (NPACK DOES NOT EQUAL NEXP)
C   IW HOLDS CHAIN COUNTER FOR OUTPUT
  IK=0
  DO 50 IN=1,NPACK
    IF(JC(IN).EQ.JCB)GO TO 40
    IK=IK+1
    IW(IK)=1
    JCB=JC(IN)
    GO TO 50
40 IW(IK)=IW(IK)+1
50 CONTINUE
  DO 60 IP=1,NPACK
    DO 60 IN=1,NEXP
      IF(IN.EQ.IC(IP))ZAS(IP)=N2(IN)
      IF(IN.EQ.IC(IP))LAMI(IP)=DUMMY(IN)
50 CONTINUE
  DO 70 IN=1,NPACK
    CALL UNPACK(ZAS(IN),Z,A,SYMB,IXCITE)
    EXCITE(IN)=BLANK
    IF(IXCITE.EQ.1)EXCITE(IN)=METAS
    SYM(IN)=SYMB
    IMASS(IN)=A
    IANO(IN)=Z
70 CONTINUE
C   *****
C   *****
C   *****
C   CALCULATE HALF-LIFE FROM LAMI (LAMI IN 1/SEC)
  DO 90 IN=1,NPACK
    IF(LAMI(IN).NE.0.0)HL(IN)=0.6931472/LAMI(IN)
90 CONTINUE
C   *****
C   *****
C   *****
C   WRITE TABLE OF PARAMETERS FOR PARENT NUCLIDES
  WRITE(IU,100)

```

```

100 FORMAT(////' RESULTS FROM DIG:  DAUGHTER INGROWTH GENERATOR'////)
      WRITE(IOUT,110)
110 FORMAT(' ORIGINAL LIST OF RADIONUCLIDES:',//,
      1 5X,'IN-LIST #',2X,'NUCLIDE',4X,'ORIG. QUANT.  TYPE',
      2 4X,'SPEC. ACT. (CI)')//
      IRK=1
      IRR=1
C     READ THE INITIAL ACTIVITIES OR MASSES FOR THE PARENTS,
C     AND THE TIME OF DECAY TB, AND OUTPUT FLAG INTERN
      READ(5,ACTIV)
      TIME=TB*SECSYR
      DO 160 IN=1,NPACK
      INDS(IN)=IN
      IF(IN.NE.IRR)GO TO 160
C     NUCLIDE IS A PARENT AND NEEDS TYPE AND QUANTITY
120 FORMAT(8X,A2,2X,E14.7)
      IF(TYPE(IR+1).NE.KG)GO TO 130
C     CONVERT FROM MASS TO SPEC. ACT.
      IF(HL(IN).NE.0.0)CONC(IN)=QUANT(IR+1)*1.128E+16/(HL(IN)*
      1                                     FLOAT(IMASS(IN)))
      GO TO 140
130 CONC(IN)=QUANT(IR+1)
140 IR=IR+1
      WRITE(IOUT,150)IR,SYM(IN),IMASS(IN),EXCITE(IN),QUANT(IR),
      1                                     TYPE(IR),CONC(IN)
150 FORMAT(7X,I3,6X,A2,'-',I3,2X,A1,2X,1PE10.3,6X,A2,6X,1PE10.3)
      IRR=IRR+IW(IRK)
      IRK=IRK+1
160 CONTINUE
C     *****
C     *****
C     CALL DECAYI TO BEGIN DECAYC CALCULATIONS - DECAY OVER TIME TB
C     CALL DECAYI(NEXP,IND,CONC,DUMMY,CRATE,VELD,IC,JC,CPAK)
C     *****
C     *****
C     SET PARAMETERS AND WRITE INTERMEDIATE TABLE IF INTERN>0
      IF(INTERN.GT.0)WRITE(IOUT,170)TB
170 FORMAT(////,' ',27('*'),' INTERMEDIATE RESULTS (INTERN > 0',
      1 ' ',27('*')),//,
      2 4X,'OUT-LIST #',2X,'NUCLIDE',2X,'ACT. (CI) AFTER',
      3 F5.1,' YRS',9X,'LAMI (1/YRS)',6X,'HALF-LIFE (YRS)')//
      IRK=1
      IRR=IW(IRK)
      INN=0
      DO 210 IN=1,NPACK
C     CONVERT HALF-LIFE (HL) AND LAMI TO 1/YEAR
      HL(IN)=HL(IN)/SECSYR
      LAMI(IN)=LAMI(IN)*SECSYR
      IF(INTERN.LT.1)GO TO 210
      IF(CONC(IN).EQ.0.0)GO TO 180
      INN=INN+1

```

```

WRITE(IOUT,200) INN, SYM(IN), IMASS(IN), EXCITE(IN),
1      CONC(IN), LAMI(IN), HL(IN)
180 CONTINUE
    IF(IN.NE. IRR)GO TO 210
    WRITE(IOUT,190)
190 FORMAT(/)
    IRK=IRK+1
    IRR=IRR+IW(IRK)
200 FORMAT(7X, I3, 6X, A2, '-', I3, A1, 9X, 1PE10.3, 16X, E10.3, 10X, E10.3)
210 CONTINUE
C *****
C *****
C DO A BUBBLE SORT ON ATOMIC NUMBERS IN ASCENDING ORDER
C FOR FINAL TABLE
    NPM1=NPACK-1
    DO 220 IN=1, NPACK
    DO 220 IP=1, NPM1
    IF(ZAS(IP).LT.ZAS(IP+1))GO TO 220
    ZTMP=ZAS(IP)
    ZAS(IP)=ZAS(IP+1)
    ZAS(IP+1)=ZTMP
    ITMP=INDS(IP)
    INDS(IP)=INDS(IP+1)
    INDS(IP+1)=ITMP
220 CONTINUE
C *****
C *****
C TOTAL ACTIVITIES BY ATOMIC NUMBER
    DO 230 IP=1, NPM1
    IF(ZAS(IP).NE.ZAS(IP+1))GO TO 230
    CONC(INDS(IP+1))=CONC(INDS(IP))+CONC(INDS(IP+1))
    INDS(IP)=0
230 CONTINUE
C *****
C *****
C WRITE FINAL TABLE
    WRITE(IOUT,240)TB
240 FORMAT(//////, ' EXPANDED LIST OF RADIONUCLIDES FROM DAUGHTER ',
1 'INGROWTH: '//5X, 'ATOMIC #', 3X, 'NUCLIDE', 2X, 'ACT. (CI) AFTER',
2 F5.1, ' YRS', 9X, 'LAMI (1/YRS)', 6X, 'HALF-LIFE (YRS)'/)
    DO 250 IN=1, NPACK
    IF(INDS(IN).EQ.0)GO TO 250
    WRITE(IOUT,200) IANO(INDS(IN)), SYM(INDS(IN)), IMASS(INDS(IN)),
1      EXCITE(INDS(IN)), CONC(INDS(IN)),
2      LAMI(INDS(IN)), HL(INDS(IN))
250 CONTINUE
C *****
    RETURN
    END
    SUBROUTINE UNPACK(ZAS, Z, A, SYMB, EXCITE)

```

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```

C      ZAS=ZAS NUMBER, A=MASS NUMBER, Z=ATOMIC NUMBER
C      THIS ROUTINE UNPACKS THE ZAS NUMBER TO FIND Z,A, AND S,
C      THE EXCITATION STATE
C      ZAS = 10000*Z + 10*A + S
C      WHERE S = 0 IF THE NUCLIDE IS IN THE NORMAL STATE
C      S = 1 WHEN IN THE EXCITATION STATE
      INTEGER A,ZAS,Z,EXCITE,ANUMBR(80)
      REAL NUCNAM(80)
      DATA NUCNAM/4HAC ,4HAG ,4HAM ,4HAR ,4HAS ,4HAT ,4HBA ,
1 4HBE ,4HBI ,4HBR ,4HBC ,4HCA ,4HCD ,4HCE ,4HCF ,
2 4HCH ,4HCO ,4HCR ,4HCS ,4HCU ,4HEU ,4HF ,4HFE ,
3 4HFR ,4HGA ,4HGD ,4HH ,4HNF ,4HNG ,4HNO ,4HI ,
4 4HIN ,4HIR ,4HK ,4HCR ,4HLA ,4HON ,4HND ,4HN ,
5 4HNA ,4HNB ,4HND ,4HNI ,4HNP ,4HO ,4HP ,4HPA ,
6 4HPB ,4HPD ,4HPM ,4HPO ,4HPR ,4HPU ,4HRA ,4HRB ,
7 4HRE ,4HRH ,4HRN ,4HRU ,4HS ,4HSB ,4HSC ,4HSE ,
8 4HSM ,4HSN ,4HSR ,4HTB ,4HTC ,4HTE ,4HTH ,4HTL ,
9 4HU ,4HV ,4HVE ,4HV ,4HZN ,4HZR ,3*4H /
      DATA ANUMBR/89,47,95,18,33,85,56,4,83,35,6,20,48,58,98,96,27,24,55
1 29,63,9,26,87,31,64,1,72,80,67,53,49,77,19,36,57,25,42,7,11,
2 41,60,28,93,8,15,91,82,46,61,84,59,94,88,37,75,45,86,44,
3 16,51,21,34,62,50,38,65,43,52,90,81,92,74,54,39,30,40,3*0/
      Z=ZAS/10000
      ITEMP=ZAS-Z*10000
      A=ITEMP/10
      EXCITE=0
      IF(MOD(ZAS,2).NE.0)EXCITE=1
      DO 100 I=1,80
      IF(Z.NE.ANUMBR(I))GO TO 100
      ISAVE=I
      GO TO 200
100 CONTINUE
      STOP 1111
200 SYMB=NUCNAM(ISAVE)
      RETURN
      END

```


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Appendix B

DIG Job Control Language

Appendix B.1. PRIMUS With DIG as a Two Step Job

```

//DASSAMPLE JOB (22620,14),'SAVE6200,160 BIN3',1,MB=3
/*ROUTE PRINT LOCAL
/*ROUTE PUNCH RMT45
/*JOBPARM COPIES=1
//A EXEC SPDASCR
//SYSIN DD *
  T.DAS22620.TTTPRIM
/*
//S1 EXEC FORTQCLG,REGION.GO=800K
//FORT.SYSPRINT DD DUMMY
//FORT.SYSIN DD *
=PRIMUS.FOR
/*
//LKED.SYSIN DD *
/*
//GO.FT06F001 DD DUMMY
//*GO.FT02F001 DD *
//GO.FT02F001 DD DISP=SHR,DSN=CAD10.OWH19503.DECAYDAT,LABEL=(,,,IN)
//GO.FT10F001 DD UNIT=SYSDA,DSN=//X,DISP=(NEW,PASS),
// SPACE=(4000,(30,8),ELSE),
// DCB=(RECFM=VBS,LRECL=X,BLKSIZE=4000)
//GO.FT12F001 DD UNIT=SYSDA,DSN=//T,DISP=(NEW,PASS),
// SPACE=(4000,(30,8),ELSE),
// DCB=(RECFM=VBS,LRECL=X,BLKSIZE=4000)
//GO.FT14F001 DD DSN=T.DAS22620.TTTPRIM,DISP=(NEW,CATLG),
// SPACE=(2000,(20,8),ELSE),UNIT=SPDA,
// DCB=(RECFM=VBS,LRECL=X,BLKSIZE=2000)
//GO.FT09F001 DD SYSOUT=A,DCB=(RECFM=FA,BLKSIZE=133)
//GO.FT03F001 DD SYSOUT=A,DEST=RMT45
//GO.FT05F001 DD *
  SAMPLE CASE

  //IOWDATA LBMODE=0,IEDIT=0,END
  //CONST NUMREL=3,END
  //NAMES REL SYM='U-238',
    'CM-242','U-235',
  //END
/*
//S2 EXEC FORTQCLG,REGION.GO=800K
//FORT.SYSPRINT DD DUMMY
//FORT.SYSIN DD *
=DIG.FOR
=DECAYC.FOR
/*
//LKED.SYSIN DD *
/*

```

```

//GO.FT14F001 DD DSN=T.DAS22620.TTIPRIM,DISP=SHR,
// SPACE=(2000,(20,8),BLSE),UNIT=SPDA,
// DCB=(RECFM=VBS,LRECL=1,BLKSIZE=2000)
//GO.FT03F001 DD SYSOUT=A,DEST=ENT45
//GO.FT05F001 DD *
  ACTIV TYPE='KG','CI','KG',QUANT=2100.,
  2.0,1.0,INTERM=1,
  TB=10.0,
  /END
/*
//
ENDINPUT

```

Appendix B.2 DIG as a One Step Job

```

//DASDIG JOB (22620,14),'SAVE6200,160 BINS',TIME=3
/*ROUTE PRINT LOCAL
/*ROUTE PUNCH RMT45
/*JOBPARM COPIES=1
// EXEC PORTQCLG,REGION.GC=800K
//PORT.SYSPRINT DD DUMMY
//PORT.SYSIN DD *
=DIG.FOR
=DECAYC.FOR
/*
//LKED.SYSIN DD *
/*
//GO.FT14F001 DD DSN=T.DAS22620.TTTPRIM,DISP=SHR.
// SPACE=(2000,(20,8),BLSE),UNIT=SPDA,
// DCB=(RECFM=VBS,LRECL=X,BLKSIZE=2000)
//GO.FT03F001 DD SYSOUT=A,DEST=RMT45
//GO.FT05F001 DD *
  ACTIV TYPE='KG','CI','KG',QUANT=2100.,
  2.0,1.0,INTERM=1,
  TB=20.0,
  END
/*
//
ENDINPUT

```

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Appendix C

Example Output Corresponding to Appendix A

Appendix C.1 Example Output from JCL in Appendix B.1

RESULTS FROM DIG: DAUGHTER INGROWTH GENERATOR

ORIGINAL LIST OF RADIONUCLIDES:

IN-LIST #	NUCLIDE	ORIG. QUANT.	TYPE	SPEC. ACT. (CI)
1	U -238	2.100E+03	KG	7.059E-01
2	CM-242	2.000E+00	CI	2.000E+00
3	U -235	1.000E+00	KG	2.161E-03

***** INTERMEDIATE RESULTS (INTERM) 0 *****

OUT-LIST #	NUCLIDE	ACT. (CI) AFTER 10.0 YRS	LAMI (1/YRS)	HALF-LIFE (YRS)
1	U -238	7.059E-01	1.551E-10	4.468E+09
2	TH-234	7.059E-01	1.050E+01	6.598E-02
3	PA-234M	7.059E-01	3.116E+05	2.225E-06
4	PA-234	1.129E-03	9.069E+02	7.643E-04
5	U -234	1.982E-05	2.835E-06	2.445E+05
6	TH-230	8.837E-10	9.002E-06	7.700E+04
7	RA-226	1.263E-12	4.332E-04	1.600E+03
8	RN-222	1.257E-12	6.621E+01	1.047E-02
9	PO-218	1.257E-12	1.195E+05	5.799E-06
10	PB-214	1.257E-12	1.360E+04	5.096E-05
11	BI-214	1.257E-12	1.832E+04	3.784E-05
12	PO-214	1.257E-12	1.336E+11	5.187E-12
13	PB-210	9.110E-14	3.114E-02	2.226E+01
14	BI-210	9.039E-14	5.050E+01	1.373E-02
15	PO-210	7.355E-14	1.830E+00	3.789E-01
16	CM-242	3.664E-07	1.551E+00	4.468E-01
17	PU-238	9.459E-03	7.899E-03	8.775E+01
18	U -234	2.603E-07	2.835E-06	2.445E+05
19	TH-230	1.115E-11	9.002E-06	7.700E+04
20	RA-226	1.527E-14	4.332E-04	1.600E+03
21	RN-222	1.520E-14	6.621E+01	1.047E-02
22	PO-218	1.520E-14	1.195E+05	5.799E-06
23	PB-214	1.519E-14	1.360E+04	5.096E-05
24	BI-214	1.519E-14	1.832E+04	3.784E-05
25	PO-214	1.519E-14	1.336E+11	5.187E-12
26	PB-210	1.059E-15	3.114E-02	2.226E+01
27	BI-210	1.050E-15	5.050E+01	1.373E-02
28	PO-210	8.476E-16	1.830E+00	3.789E-01
29	U -235	2.161E-03	9.848E-10	7.038E+08
30	TH-231	2.161E-03	2.381E+02	2.911E-03
31	PA-231	4.018E-07	1.860E-05	3.726E+04

32	AC-227	5.766E-08	3.183E-02	2.177E+01
33	FR-223	7.957E-10	1.672E+04	4.145E-05
34	TH-227	5.607E-08	1.353E+01	5.125E-02
35	RA-223	5.638E-08	2.214E+01	3.131E-02
36	RN-219	5.638E-08	5.524E+06	1.255E-07
37	PO-215	5.638E-08	1.230E+10	5.634E-11
38	FB-211	5.637E-08	1.010E+04	6.864E-05
39	BI-211	5.637E-08	1.712E+05	4.050E-06
40	PO-211	1.539E-10	4.239E+07	1.635E-08
41	TL-207	5.622E-08	7.643E+04	9.069E-06

EXPANDED LIST OF RADIONUCLIDES FROM DAUGHTER INGROWTH:

ATOMIC #	NUCLIDE	ACT. (CI) AFTER 10.0 YRS	LANI (1/YRS)	HALF-LIFE (YRS)
81	TL-207	5.622E-08	7.643E+04	9.069E-06
82	FB-210	9.216E-14	3.114E-02	2.226E+01
82	FB-211	5.637E-08	1.010E+04	6.864E-05
82	FB-214	1.272E-12	3.60E+04	5.096E-05
83	BI-210	9.144E-14	5.150E+01	1.373E-02
83	BI-211	5.637E-08	1.712E+05	4.050E-06
83	BI-214	1.272E-12	1.832E+04	3.784E-05
84	PO-210	7.439E-14	1.830E+00	3.789E-01
84	PO-211	1.539E-10	4.239E+07	1.635E-08
84	PO-214	1.272E-12	1.336E+11	5.187E-12
84	PO-215	5.638E-08	1.230E+10	5.634E-11
84	PO-218	1.272E-12	1.195E+05	5.799E-06
86	RN-219	5.638E-08	5.524E+06	1.255E-07
86	RN-222	1.272E-12	6.621E+01	1.047E-02
87	FR-223	7.957E-10	1.672E+04	4.145E-05
88	RA-223	5.638E-08	2.214E+01	3.131E-02
88	RA-226	1.278E-12	4.332E-04	1.600E+03
89	AC-227	5.766E-08	3.183E-02	2.177E+01
90	TH-227	5.607E-08	1.353E+01	5.125E-02
90	TH-230	8.948E-10	9.002E-06	7.700E+04
90	TH-231	2.161E-03	2.381E+02	2.911E-03
90	TH-234	7.059E-01	1.050E+01	6.598E-02
91	PA-231	4.018E-07	1.860E-05	3.726E+04
91	PA-234	1.129E-03	9.069E+02	7.643E-04
91	PA-234M	7.059E-01	3.116E+05	2.225E-06
92	U -234	2.008E-05	2.835E-06	2.445E+05
92	U -235	2.161E-03	9.848E-10	7.038E+08
92	U -238	7.059E-01	1.551E-10	4.468E+09
94	PU-238	9.459E-03	7.899E-03	6.775E+01
96	CM-242	3.664E-07	1.551E+00	4.468E-01

Appendix C.2 Example Output from JCL in Appendix B.2

RESULTS FROM DIG: DAUGHTER INGROWTH GENERATOR

ORIGINAL LIST OF RADIONUCLIDES:

IN-LIST #	NUCLIDE	ORIG. QUANT.	TYPE	SPEC. ACT. (CI)
1	U -238	2.100E+03	KG	7.059E-01
2	CN-242	2.000E+00	CI	2.000E+00
3	U -235	1.000E+00	KG	2.161E-03

***** INTERMEDIATE RESULTS (INTERM > 0) *****

OUT-LIST #	NUCLIDE	ACT. (CI) AFTER 20.0 YRS	LAMI (1/YRS)	HALF-LIFE (YRS)
1	U -238	7.059E-01	1.551E-10	4.468E+03
2	TH-234	7.059E-01	1.050E+01	6.598E-02
3	PA-234M	7.059E-01	3.116E+05	2.225E-06
4	PA-234	1.129E-03	9.069E+02	7.643E-04
5	U -234	3.983E-05	2.835E-06	2.445E+05
6	TH-230	3.568E-09	9.002E-06	7.700E+04
7	RA-226	1.023E-11	4.332E-04	1.600E+03
8	RN-222	1.021E-11	6.621E+01	1.047E-02
9	PO-218	1.021E-11	1.195E+05	5.799E-06
10	PB-214	1.021E-11	1.360E+04	5.096E-05
11	BI-214	1.021E-11	1.832E+04	3.784E-05
12	PO-214	1.021E-11	1.336E+11	5.187E-12
13	PB-210	1.404E-12	3.114E-02	2.226E+01
14	BI-210	1.398E-12	5.050E+01	1.373E-02
15	PO-210	1.260E-12	1.830E+00	3.789E-01
16	CN-242	6.713E-14	1.551E+00	4.468E-01
17	PU-238	8.740E-03	7.899E-03	8.775E+01
18	U -234	5.181E-07	2.835E-06	2.445E+05
19	TH-230	4.633E-11	9.002E-06	7.700E+04
20	RA-226	1.311E-13	4.332E-04	1.600E+03
21	RN-222	1.308E-13	6.621E+01	1.047E-02
22	PO-218	1.308E-13	1.195E+05	5.799E-06
23	PB-214	1.308E-13	1.360E+04	5.096E-05
24	BI-214	1.308E-13	1.832E+04	3.784E-05
25	PO-214	1.308E-13	1.336E+11	5.187E-12
26	PB-210	1.771E-14	3.114E-02	2.226E+01
27	BI-210	1.764E-14	5.050E+01	1.373E-02
28	PO-210	1.587E-14	1.830E+00	3.789E-01

29	U -235	2.161E-03	9.848E-10	7.038E+08
30	TH-231	2.161E-03	2.381E+02	2.911E-03
31	PA-231	8.037E-07	1.860E-05	3.726E+04
32	AC-227	2.092E-07	3.183E-02	2.177E+01
33	FR-223	2.887E-09	1.672E+04	4.145E-05
34	TH-227	2.049E-07	1.353E+01	5.125E-02
35	RA-223	2.070E-07	2.214E+01	3.131E-02
36	RN-219	2.070E-07	5.524E+06	1.255E-07
37	PO-215	2.070E-07	1.230E+10	5.634E-11
38	FB-211	2.070E-07	1.010E+04	6.864E-05
39	BI-211	2.070E-07	1.712E+05	4.050E-06
40	PO-211	5.650E-10	4.239E+07	1.635E-08
41	TL-207	2.064E-07	7.643E+04	9.069E-06

EXPANDED LIST OF RADIONUCLIDES FROM DAUGHTER INGROWTH:

ATOMIC #	NUCLIDE	ACT. (CI) AFTER 20.0 YRS	LAMI (1/YRS)	HALF-LIFE (YRS)
81	TL-207	2.064E-07	7.643E+04	9.069E-06
82	FB-210	1.422E-12	3.114E-02	2.226E+01
82	FB-211	2.070E-07	1.010E+04	6.864E-05
82	FB-214	1.034E-11	1.360E+04	5.096E-05
83	BI-210	1.416E-12	5.050E+01	1.373E-02
83	BI-211	2.070E-07	1.712E+05	4.050E-06
83	BI-214	1.034E-11	1.832E+04	3.784E-05
84	PO-210	1.276E-12	1.830E+00	3.789E-01
84	PO-211	5.650E-10	4.239E+07	1.635E-08
84	PO-214	1.034E-11	1.336E+11	5.187E-12
84	PO-215	2.070E-07	1.230E+10	5.634E-11
84	PO-218	1.034E-11	1.195E+05	5.799E-06
86	RN-219	2.070E-07	5.524E+06	1.255E-07
86	RN-222	1.034E-11	6.621E+01	1.047E-02
87	FR-223	2.887E-09	1.672E+04	4.145E-05
88	RA-223	2.070E-07	2.214E+01	3.131E-02
88	RA-226	1.037E-11	4.332E-04	1.600E+03
89	AC-227	2.092E-07	3.183E-02	2.177E+01
90	TH-227	2.049E-07	1.353E+01	5.125E-02
90	TH-230	3.615E-09	9.002E-06	7.700E+04
90	TH-231	2.161E-03	2.381E+02	2.911E-03
90	TH-234	7.059E-01	1.050E+01	6.598E-02
91	PA-231	8.037E-07	1.860E-05	3.726E+04
91	PA-234	1.129E-03	9.069E+02	7.643E-04
91	PA-234M	7.059E-01	3.116E+05	2.225E-06
92	U -234	4.035E-05	2.835E-06	2.445E+05
92	U -235	2.161E-03	9.848E-10	7.038E+08
92	U -238	7.059E-01	1.551E-10	4.468E+09
94	PU-238	8.740E-03	7.899E-03	8.775E+01
96	CM-242	6.713E-14	1.551E+00	4.468E-01

Appendix D

DCHAIN — A Program to Unpack PRIMUS Data Sets

This appendix contains a FORTRAN listing of code DCHAIN, the job control language, and a sample output from using DCHAIN. DCHAIN is a program which may be used to unpack (from compressed data format) and display the PRIMUS data set generated in Step 1, described in Chapter 2. This program is included as a convenience to those who may wish to make use of the radionuclide data set in other applications.

Appendix D.1 DCHAIN Code Listing

```

REAL*8 SYMK, SYMJ                                MAIN0010
INTEGER A, EXCITE, Z, ZAS                          MAIN0020
DIMENSION SYM(200), IMASS(200), IXCITE(200), JINL(200), ZAS(200)  MAIN0030
DIMENSION NI(200), NZ(200), IC(200), JC(200), S(37,37)  MAIN0040
DATA NPRIME/11/, IOUT/3/                          MAIN0050
REWIND NPRIME                                       MAIN0060
READ (NPRIME) NUNCHA, KTRUNC, NPACK                MAIN0070
READ(NPRIME)(IC(N), N=1, NPACK), (JC(I), I=1, NPACK)  MAIN0080
READ(NPRIME)                                       MAIN0090
READ(NPRIME) NREL, NEXP, (NI(J), J=1, NREL), (NZ(I), I=1, NEXP)  MAIN0100
WRITE(IOUT,800)                                    MAIN0110
DO 100 IN=1, NREL                                  MAIN0120
CALL UNPACK(NI(IN), Z, A, SYMB, EXCITE)             MAIN0130
IF(EXCITE.EQ.0) WRITE(IOUT,1000) IN, SYMB, A        MAIN0140
IF(EXCITE.EQ.1) WRITE(IOUT,1100) IN, SYMB, A        MAIN0150
100 CONTINUE                                       MAIN0160
WRITE(IOUT,900)                                    MAIN0170
DO 200 IN=1, NEXP                                  MAIN0180
CALL UNPACK(NZ(IN), Z, A, SYMB, EXCITE)             MAIN0190
IF(EXCITE.EQ.0) WRITE(IOUT,1000) IN, SYMB, A        MAIN0200
IF(EXCITE.EQ.1) WRITE(IOUT,1100) IN, SYMB, A        MAIN0210
200 CONTINUE                                       MAIN0220
STOP                                                MAIN0230
800 FORMAT(' ORIGINAL LIST OF RADIONUCLIDES:', //,   MAIN0240
1 5X, 'IN-LIST #', 2X, 'NUCLIDE', /)                MAIN0250
900 FORMAT(////, ' EXPANDED LIST OF RADIONUCLIDES FROM DAUGHTER INGROWTH' MAIN0260
1H: ', /, 4X, 'OUT-LIST #', 2X, 'NUCLIDE', /)        MAIN0270
1000 FORMAT(7X, I3, 6X, A2, '- ', I3)               MAIN0280
1100 FORMAT(7X, I3, 6X, A2, '- ', I3, 'M')           MAIN0290
END                                                  MAIN0300
SUBROUTINE UNPACK(ZAS, Z, A, SYMB, EXCITE)          UNPC0010
C   ZAS=ZAS NUMBER, A=MASS NUMBER, Z=ATOMIC NUMBER  UNPC0020
C   THIS ROUTINE UNPACKS THE ZAS NUMBER TO FIND Z, A, AND S,  UNPC0030
C   THE EXCITATION STATE                                UNPC0040
C   ZAS = 10000*Z + 10*A + S                          UNPC0050
C   WHERE S = 0 IF THE NUCLIDE IS IN THE NORMAL STATE  UNPC0060
C   S = 1 WHEN IN THE EXCITATION STATE                UNPC0070
C   INTEGER A, ZAS, Z, EXCITE, ANUMBR(80)             UNPC0080
REAL NUCNAM(80)                                     UNPC0090
DATA NUCNAM/4HAC ,4HAG ,4HAM ,4HAR ,4HAS ,4HAT ,4HBA ,  UNPC0100
1 4HBE ,4HBI ,4HBR ,4HC ,4HCA ,4HCD ,4HCE ,4HCF ,  UNPC0110
2 4HCM ,4HCO ,4HCR ,4HCS ,4HCU ,4HEU ,4HF ,4HFE ,  UNPC0120
3 4HFR ,4HGA ,4HGD ,4HH ,4HHF ,4HHG ,4HHO ,4HI ,  UNPC0130
4 4HIN ,4HIR ,4HK ,4HXR ,4HLA ,4HMA ,4HMO ,4HN ,  UNPC0140
5 4HNA ,4HNB ,4HND ,4HNI ,4HNP ,4HO ,4HP ,4HPA ,  UNPC0150

```

6	4HPB	,4HPD	,4HPM	,4HPO	,4HPR	,4HPU	,4HRA	,4HRS		UNPC0160
7	4HRE	,4HRH	,4HRN	,4HRU	,4HS	,4HSB	,4HSC	,4HSE		UNPC0170
8	4HSM	,4HSN	,4HSR	,4HTB	,4HTC	,4HTE	,4HTH	,4HTL		UNPC0180
9	4HU	,4HW	,4HXB	,4HY	,4HZN	,4HZR	,3*4H	/		UNPC0190
	DATA ANUMBR/89,47,95,18,33,85,56,4,83,35,6,20,48,58,98,96,27,24,55									UNPC0200
	1,29,53,9,26,87,31,64,1,72,80,67,53,49,77,19,36,57,25,42,7,11,									UNPC0210
2	41,60,28,93,8,15,91,82,46,61,84,59,94,88,37,75,45,86,44,									UNPC0220
3	16,51,21,34,62,50,38,65,43,52,90,81,92,74,54,39,30,40,3*0/									UNPC0230
	Z=ZAS/10000									UNPC0240
	ITEMP=ZAS-Z*10000									UNPC0250
	A=ITEMP/10									UNPC0260
	EXCITE=0									UNPC0270
	IF(MOD(ZAS,2).NE.0)EXCITE=1									UNPC0280
	DO 100 I=1,80									UNPC0290
	IF(Z.NE.ANUMBR(I))GO TO 100									UNPC0300
	ISAVE=I									UNPC0310
	GO TO 200									UNPC0320
100	CONTINUE									UNPC0330
	STOP 1111									UNPC0340
200	SYMB=NUCNAM(ISAVE)									UNPC0350
	RETURN									UNPC0360
	END									UNPC0370

Appendix D.2 DCHAIN Job Control Language

```

//DASDEC JOB (22620,101), 'SAVE6200,160 BIN-S', TIME=(0,20)
/*JOBPARM LINES=20, COPIES=1
/*RCOTE PRINT LOCAL
// EXEC FORTDCLG, PARM.FORT='XREF', PARM.GO='DIMP=G, EU=-1',
// REGION.GO=350K
/*FORT.SYSPRINT DD DUMMY
//FORT.SYSIN DD *
=DCHAIN.FOR
/*
/*LKED.SYSPRINT DD DUMMY
//LKED.SYSIN DD *
/*
//GO.FT03F001 DD SYSOUT=A, DEST=EMT45
//GO.FT11F001 DD UNIT=SPDA, DISP=SHR, DSN=T.DAS22620.TTTPRIM
/*
//
ENDINPUT

```

Appendix D.3. Example Output from DCHAIN

ORIGINAL LIST OF RADIONUCLIDES:

IN-LIST # NUCLIDE

1	U -238
2	CM-242
3	U -235

EXPANDED LIST OF RADIONUCLIDES FROM DAUGHTER INGROWTH:

OUT-LIST # NUCLIDE

1	U -238
2	TH-234
3	PA-234M
4	PA-234
5	CM-242
6	PU-238
7	U -234
8	TH-230
9	RA-226
10	KN-222
11	PO-218
12	PB-214
13	BI-214
14	PO-214
15	PB-210
16	BI-210
17	PO-210
18	U -235
19	TH-231
20	PA-231
21	AC-227
22	FR-223
23	TH-227
24	RA-223
25	KN-219
26	PO-215
27	PB-211
28	BI-211
29	PO-211
30	TL-207

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